

# Heatbath Noise Methods in Lattice QCD

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In a recent paper, de Forcrand has pointed out that matrix inversions using Gaussian noise need not be iterated to full convergence, but instead may be solved approximately and treated as a heatbath. Gaussian noise however is not optimal for minimizing variance. It shown here how his algorithm may be generalized to a mixture of Gaussian and Z(N) noise, resulting in a smaller effective variance for some operators.

## 1. Introduction

Usually, one solves  $A\vec{\phi} = \vec{\eta}$ , where  $\vec{\eta}$  is a noise vector, to full convergence. DeForcrand pointed out[1] that this is not necessary for Gaussian noise. Formally,

$$\langle \mathcal{O} \rangle = \frac{1}{Z_\phi} \int D\vec{\phi} e^{-|A\vec{\phi}|^2} \mathcal{O}. \quad (1)$$

Introduce an auxilliary field,

$$\langle \mathcal{O} \rangle = \frac{1}{\pi^N Z_\phi} \int D\vec{\chi} \int D\vec{\phi} e^{-|A\vec{\phi}|^2 - |\vec{\chi} - A\vec{\phi}|^2} \mathcal{O}. \quad (2)$$

Consider a change,

$$\vec{\phi} \rightarrow \vec{\phi}'; \vec{\phi}' = \vec{\zeta} - \vec{\phi}, A\vec{\zeta} = \vec{\chi} - \vec{r}, \vec{\chi} = A\vec{\phi} + \vec{\eta}, \quad (3)$$

where  $\vec{\eta}$  is a complex Gaussian noise vector and  $\vec{r}$  is the residual vector in the solution for  $\vec{\phi}'$ . One can show the change is accepted with probability

$$P_A(\vec{\phi} \rightarrow \vec{\phi}') = \min(1, e^{-\Delta S}), \quad (4)$$

where

$$\begin{aligned} \Delta S &= |A\vec{\phi}'|^2 + |\vec{\chi} - A\vec{\phi}'|^2 - |A\vec{\phi}|^2 - |\vec{\chi} - A\vec{\phi}|^2, \\ &= 2\text{Re}(\vec{r}^\dagger \cdot A(\vec{\phi} - \vec{\phi}')). \end{aligned} \quad (5)$$

With the assumption that  $A\vec{\phi}$ ,  $A\vec{\phi}'$ , and  $\vec{r}$  are uncorrelated Gaussian vectors of variance  $N$ ,  $N$  and  $\epsilon^2 N$  respectively ( $N$  is the dimensionality of  $A$ ), DeForcrand shows that

$$P_A(\vec{\phi} \rightarrow \vec{\phi}') \approx \text{erfc}\left(\epsilon \sqrt{\frac{N}{2}}\right). \quad (6)$$

( $\epsilon \equiv \frac{||\vec{r}||}{||A\vec{\phi}'||}$ ) The computational overhead is simply one matrix-vector product plus several matrix

dot products per acceptance check. This can save a factor of 2 to 3 in computer time. This is the general idea; generalizations are also presented by DeForcrand.

## 2. Accelerating Z(N) Noise

Gaussian noise is not optimal for signal extraction[2]. Therefore it is of interest to see if heatbath methods can be adapted to use a mixture of Gaussian and Z(N) noise (Z(2) used here).

For this purpose, we begin with the expression,

$$\langle \mathcal{O} \rangle = \frac{1}{Z_\phi a^{2N} \mathcal{N}} \sum_i \int D\vec{\phi} e^{-\frac{1}{a^2} |A\vec{\phi} - b\vec{Z}^i|^2} \mathcal{O}, \quad (7)$$

where  $\vec{Z}^i$  is a particular Z(2) noise vector and  $\mathcal{N} = 2^N$  is the number of Z(2) noises in the vector space and  $a^2 + b^2 = 1$ . Let  $\mathcal{O} = \sum_{ij} \phi_j^\dagger A_{ji}^\dagger \phi_i$ . One can do the integrals to get,

$$\begin{aligned} \langle \phi_j^\dagger A_{ji}^\dagger \phi_i \rangle &= \frac{1}{\mathcal{N}} \sum_i [a^2 \sum_j A_{jj}^{-1} + \\ &\quad b^2 \sum_{j,k} Z_j^i A_{jk}^{-1} Z_k^i]. \end{aligned} \quad (8)$$

Then with

$$\frac{1}{\mathcal{N}} \sum_i Z_j^i Z_k^i = \delta_{jk}, \quad (9)$$

we see that the answer is just  $\text{Tr} A^{-1}$ , but with a weighting over Gaussian ( $a^2$ ) and Z(2) ( $b^2$ ) noises. We introduce  $\vec{\chi}$  as before,

$$\begin{aligned} \langle \mathcal{O} \rangle &= \frac{1}{(\pi a^4)^N Z_\phi \mathcal{N}} \int D\vec{\chi} \sum_i \int D\vec{\phi} \\ &\quad e^{-\frac{1}{a^2} |A\vec{\phi} - b\vec{Z}^i|^2 - \frac{1}{a^2} |\vec{\chi} - A\vec{\phi} + b\vec{Z}^i|^2} \mathcal{O}, \end{aligned} \quad (10)$$

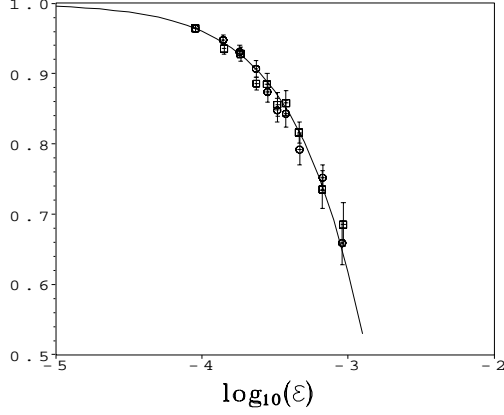


Figure 1. The acceptance,  $P_A$ , as a function of  $\log_{10}(\epsilon)$  for  $b/a = 0$  (boxes) and  $b/a = 1$  (circles).

treating  $\vec{Z}^i$  as a dynamical variable, the change in the action is now,

$$\Delta S = \frac{1}{a^2} [ |A\vec{\phi}' - b\vec{Z}^{i'}|^2 + |\vec{\chi} - A\vec{\phi}' + b\vec{Z}^{i'}|^2 - |A\vec{\phi} - b\vec{Z}^i|^2 - |\vec{\chi} - A\vec{\phi} + b\vec{Z}^i|^2 ]. \quad (11)$$

This is again a heatbath, with

$$\Delta S = 2\text{Re}(\vec{r}^{a\dagger} \cdot (A^a\vec{\phi} - \frac{b}{a}\vec{Z}^i - A^a\vec{\phi}' + \frac{b}{a}\vec{Z}^{i'})), \quad (12)$$

where  $A^a \equiv A/a$  and  $\vec{r}^a \equiv \vec{r}/a$ . This is of the same form as above and has the same acceptance since  $(A^a\vec{\phi} - \frac{b}{a}\vec{Z}^i)$  and  $(A^a\vec{\phi}' - \frac{b}{a}\vec{Z}^{i'})$  have variance  $N$ . The rescaled  $\vec{r}^a$  is used to define the residual,  $\epsilon$ , in the computer program.

Although the acceptance is the same, the number of iterations is greater for a given cutoff,  $\epsilon$ , on the new residual vector since it is defined by dividing by  $a < 1$ . However, since the convergence on the residual is typically exponential, changes in  $a$  are accommodated by a modest number of extra iterations. The fact that the acceptance is the same at the rescaled  $\epsilon$  value we will see has the helpful consequence that one does not have to re-search for the optimum  $\epsilon$  value at which to run, even though now we use a noise mixture.

The above discussion can be generalized to justify more complicated exponential shifts  $A\vec{\phi} \rightarrow$

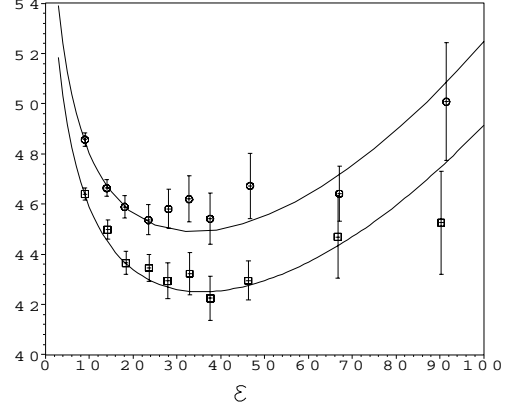


Figure 2. The number of mixed Z(2)/Gaussian heatbath iterations divided by the model acceptance,  $N_{mixed}/P_A$ , as a function of  $\epsilon$  in units of  $10^{-5}$  for  $b/a = 0$  (boxes) and  $b/a = 1$  (circles).

$A\vec{\phi} - \vec{C}^i$  where  $\vec{C}^i$  can depend on other noises, parameters, etc., besides the specific one  $\vec{C}^i = b\vec{Z}^i$  used above. I am using a solver which has enforced even/odd preconditioning in the Wilson/Dirac matrix  $M$ . One can show that in this case one is not simulating  $A = M$  directly as in the above discussion, but a different, shifted system and the residual vector is purely in one sector (even/odd) or the other.

Figs. 1 and 2 show acceptance data on a  $12^3 \times 24$  lattice using the Wilson/Dirac matrix at  $\kappa = 0.148$ . I am calculating the average acceptance on 100 noises at various cutoff values of  $\epsilon$  and with  $b/a = 0$  and 1. For this solver I get about a 6% increase in the number of iterations for this ratio. (The model suggests about 14% increase in the number of iterations for an 80% mixture ( $b/a = 2$ ) and about a 30% increase for a 97.3% mixture ( $b/a = 6$ ) for the parameters in this simulation.) Fig. 1 shows  $P_A$  in the crucial window of  $\epsilon$  of from  $10^{-4}$  through  $10^{-3}$ , where it varies between  $\sim 0.97$  to  $0.65$  for  $b/a = 0, 1$  for a single gauge configuration. The acceptance is the same for both  $b/a$  values within errors and agrees with Eq.(6). The reason this interval is crucial is illus-

trated in Fig. 2. There we see that the number of mixed Z(2)/Gaussian heatbath iterations divided by the acceptance,  $N_{mixed}/P_A$ , has a minimum at  $\epsilon \sim 4 \times 10^{-4}$  for  $b/a = 0, 1$ . Shown here also is the model value for this quantity given by

$$N_{mixed}/P_A = \frac{-\frac{1}{c} \ln(a\epsilon \frac{\sqrt{N}}{r_0})}{\text{erfc}(\epsilon \sqrt{\frac{N}{2}})}, \quad (13)$$

where  $N_{mixed}$  is assumed determined by  $||\vec{r}|| = r_0 e^{-cN_{mixed}}$ . As noted above, I am using a solver which has enforced even/odd preconditioning in the Wilson/Dirac matrix  $M$ . The upshot for this simulation is that  $N$  in (6) and (13) must include a factor of  $\frac{1}{2}$ ,  $N = \frac{1}{2} \times (12^3 \times 24 \times 4 \times 3)$ .

Fig.3 shows the normed effective mixed Z(2)/Gaussian variance in the operator  $\bar{\psi}\psi$  as a function of  $b/a$ . It has a very shallow minimum at  $b/a \approx 10$ . By normed effective variance I mean the ratio  $(V_{mixed} \times N_{mixed})/(V_{Gauss} \times N_{Gauss})$ , which takes into account that  $N_{mixed} > N_{Gauss}$  for  $b \neq 0$ . The model and data suggest that the minimum of this ratio is  $\approx 0.3$ . The horizontal line gives the fully converged value of the variance ratio  $V_{Z(2)}/V_{Gauss}$ , which is  $\approx 0.2$ . Thus, one loses a factor of  $\approx 2/3$  in the effective variance compared to the fully converged Z(2) simulation. The gain in computer time is reduced from a factor of from 2 to 3 to a factor of from 1.33 to 2. These numbers are apparently typical. Other operators with larger converged  $V_{Z(2)}/V_{Gauss}$  ratios have sharper minima at smaller  $b/a$ .

### 3. Conclusions and Observations

Ref.[1] shows that heatbath methods can speed up simulations of many disconnected loop operators or by a factor of  $\approx 2$  to 3. However, Gaussian noise is not optimal and so heatbath methods do not help for operators whose variance is diagonally dominate, such as Wilson  $\bar{\psi}\psi$ . It has been shown here that these methods can be generalized to a mixture of Gaussian and Z(N) noise. With an mixture/iteration penalty factor of about 2/3, the Gaussian noise accelerates the Z(N) sector.

For diagonally dominate operators, there exists a Z(N)/Gaussian ratio that minimizes the variance. The noise can then be tailored to the opera-

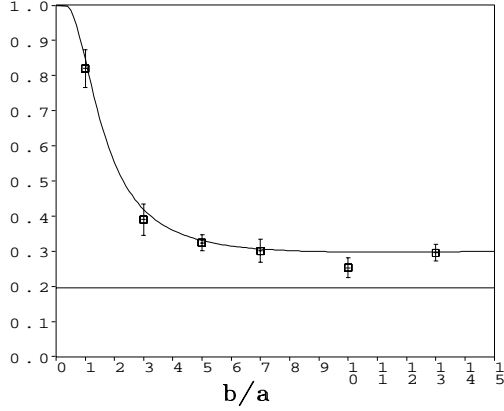


Figure 3. Effective variance of the  $b \neq 0$  simulation for  $\bar{\psi}\psi$  normalized to the Gaussian simulation with  $b = 0$  as a function of  $b/a$ .

tor (“designer noise”). The optimum  $b/a$  parameter can be numerically estimated from the parameters of the model and an independent measurement of the fully converged Z(N)/Gaussian variance ratio.

It is not shown here, but the even/odd structure of the Wilson/Dirac matrix can be exploited to increase the computer time gain of diagonally dominate operators further by restricting the Gaussian noise to only one sector or the other. This and other aspects of heatbath noise methods will be discussed in a future publication.

### 4. Acknowledgements

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